

Robustness of the optical-conductivity sum rule in Bilayer Graphene

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(Dated: April 8, 2008)

We calculate the optical sum associated with the in-plane conductivity of a graphene bilayer. A bilayer asymmetry gap generated in a field-effect device can split apart valence and conduction bands, which otherwise would meet at two \mathbf{K} points in the Brillouin zone. In this way one can go from a compensated semimetal to a semiconductor with a tunable gap. However, the sum rule turns out to be 'protected' against the opening of this semiconducting gap, in contrast to the large variations observed in other systems where the gap is induced by strong correlation effects.

I. INTRODUCTION

Sum rules on the conductivity have played an important role in the analysis of optical conductivity data, which give information on electron dynamics. In its simplest form, for an infinite free electron band, the sum rule gives the plasma frequency which is independent of temperature, interactions and impurity scattering.^{1,2} In tight-binding models it is related to the second derivative with respect to the momentum $k_{x,y}$ of the band dispersion $\varepsilon_{\mathbf{k}}$, times the probability of occupation of the state $|\mathbf{k}\rangle$.^{1,2} In the special case where only nearest-neighbor hopping is present on a square lattice, the sum-rule integral reduces to minus one half the kinetic energy in appropriate units. As a consequence, in general it is affected by the interactions present in the system, and these determine both its absolute value and its variations with temperature. This fact has been investigated recently both experimentally and theoretically in the context of high- T_c cuprate superconductors (see Ref. [1,2] for a review). It follows from the Sommerfeld expansion that the relative temperature variation of the sum-rule integral in non-interacting tight-binding models is proportional to $(T/t)^2$, where t is the nearest-neighbor hopping. In the experiments done in the normal state of cuprates, the temperature variations of the the sum rule are much larger than this estimate, and in some cases deviate from a simple T^2 law. The discrepancy can be attributed to correlation effects. For example, in the studies of the Hubbard or $t - J$ model^{3,4}, a new energy scale emerges associated with the reduced width of the renormalized band. This parameter replaces the hopping parameter t in the $(T/t)^2$ dependence leading to its enhancement. It is shown in other theoretical approaches that the sum rule integral measures instead a specific average of the quasiparticle lifetime⁵⁻⁸ normalized to the Fermi energy ε_F , and hence such optical experiments ultimately probe correlation effects through lifetime broadening. These examples illustrate that optical data can provide important insight into correlation effects.

Graphene, which is a single layer of graphite, has recently been isolated and its properties investigated (see Ref. 9 for a review). Bilayer graphene¹⁰ and thicker

graphite films are also now widely produced. Since graphene possesses truly remarkable properties both from the technological and theoretical points of view, there has already been considerable work done on monolayer and bilayer graphene and also on related materials. In particular, recent data are available on the AC conductivity in the infrared region of graphite^{11,12}, several layer epitaxial graphite¹³, and on monolayer¹⁴ and bilayer¹⁵ graphene. There has also been much theoretical work on the microwave and infrared conductivity of graphene¹⁶⁻¹⁸ (see Ref. 19 for a review) and on a bilayer²⁰⁻²² and multilayer.^{18,23} Thus, it is of interest to anticipate some general results on the optical-conductivity sum rule behavior of these systems, which are likely to be tested experimentally in the near future. The optical sum rules for the (in-plane) longitudinal and Hall conductivities were studied for monolayer graphene in Ref.[24], where the unusual dependences of the sum rules on temperature and chemical potential were revealed. For example, at the neutral Dirac point the linear dispersion law of quasiparticles leads to a T^3 dependence of the sum-rule, instead of the T^2 law found in tight-binding bands^{1,2}.

A specific and very useful feature of graphene, not available in ordinary metals, is that it is possible to change the chemical potential μ and thus the number of carriers by tuning the gate voltage V_g ($V_g \propto \mu^2$ for monolayer graphene) in a field-effect device. It was shown²⁴ that in the limit $T = 0$ the concentration-dependent part of the sum rule goes like $(|\mu|/t)^3$. For a finite temperature $T \ll |\mu|$, there is a temperature dependent correction to the sum of order $(|\mu|/t)(T/t)^2$ which is very much as in the more ordinary T^2 -law case discussed above.

In this paper we generalize the previous work to the case of bilayer graphene. In the case considered most often, a bilayer graphene consists of two coupled hexagonal lattices. The inequivalent sites A1, B1 and A2, B2 on the bottom and top graphene sheets are arranged according to Bernal (A2-B1) stacking: every B1 site in the bottom layer lies directly below an A2 site in the upper layer. The strongest inter-layer coupling between pairs of A2 - B1 orbitals, γ_1 , changes the electron dispersion from a linear to a quadratic form^{21,25}. In addition to this effect, bilayer graphene is the only known material in which the elec-

tronic band structure can be changed significantly simply by applying an electric field perpendicular to the layers.⁹ Indeed, while the unbiased bilayer system is a semi-metal, with parabolic valence and conduction band touching each other at the neutrality point, the system becomes a semiconductor when the two layers are electrostatically inequivalent. The corresponding semiconducting gap Δ between valence and conduction bands is tunable continuously from zero to ≈ 0.2 eV.^{9,26,27} As shown experimentally, the asymmetry gap Δ and the carrier concentration can be controlled independently through an applied gate voltage and chemical deposition of potassium or other atoms on the vacuum side of the structure.^{26,27} Recently, similar results have also been obtained in a double-gated structure made of bilayer graphene sandwiched in between two gate electrodes²⁸. This effect has been understood by means of both tight-binding calculations^{26,29,30} and ab initio calculations³¹.

Beyond the clear potential impact that this effect has on device applications, it is extremely interesting from the theoretical point of view to understand how this field-induced band transition will affect the conduction properties of the system. In light of the previous discussion concerning the physics of cuprates, one could ask if the opening of the gap due to the metal-insulator transition in Hubbard-like models, or across the metal-superconductor transition in superconducting models, share commonality with the physics of bilayer graphene. As we shall demonstrate below, these phenomena are drastically different. Indeed, we show that the sum rule is essentially protected against the opening of the semiconductor gap in this bilayer system. Despite the fact that Δ can be as big as a significant fraction of the Fermi energy, the relative sum-rule changes from the unbiased to the biased system are of order of 10^{-3} . Thus, even though a general redistribution of spectral weight is expected due to the opening of the gap, the total sum rule is practically constant. One would have expected the large band structure changes involved to lead to corresponding significant changes in the optical sum. Here, however, we show that this is not the case. The relative changes in optical spectral weight induced by the opening of the gap must largely compensate each other, leaving the total weight almost unchanged.

II. DERIVATION OF THE SUM RULE

For a generic electronic model described by the Hamiltonian H the optical-conductivity sum rule is given by:^{1,2}

$$W(T) = \int_{-\infty}^{\infty} \text{Re} \sigma_{xx}(\omega) d\omega = \frac{\pi e^2}{\mathcal{V}} \langle \tau_{xx} \rangle, \quad (1)$$

where \mathcal{V} is the unit-cell volume and τ_{xx} is the so-called mass tensor, which appears in the second-order expansion

of H evaluated at finite vector potential \mathbf{A} :

$$H(\mathbf{A}) \approx H(0) - \sum_{\mathbf{n}, \alpha=x,y} \left[\frac{e}{c} A_{\alpha}(\mathbf{n}) j_{\alpha}(\mathbf{n}) - \frac{e^2}{2c^2} A_{\alpha}^2(\mathbf{n}) \tau_{\alpha\alpha}(\mathbf{n}) \right], \quad (2)$$

and j_{α} is the current density in the α direction. The vector potential \mathbf{A} is introduced in the tight-binding Hamiltonian (3) written below by means of the Peierls substitution, $a_{2\mathbf{n}}^{\dagger} b_{2\mathbf{n}+\boldsymbol{\delta}'} \rightarrow a_{2\mathbf{n}}^{\dagger} \exp\left(-\frac{ie}{\hbar c} \int_{\mathbf{n}+\boldsymbol{\delta}'}^{\mathbf{n}} \mathbf{A} d\mathbf{r}\right) b_{2\mathbf{n}+\boldsymbol{\delta}'}$. Here $a_{2\mathbf{n}}$ and $b_{2\mathbf{n}+\boldsymbol{\delta}'}$ are the Fermi operators of electrons on A2, B2 sublattices of the second layer. (Note that this Peierls substitution corresponds to the 2nd layer, for the 1st layer it is similar. The spin label is omitted.) The positions of A2 and B1 atoms are denoted as \mathbf{n} and they are connected to their nearest neighbors on B2 (A1) sites by the three vectors $\boldsymbol{\delta}'$ ($\boldsymbol{\delta}$). Accordingly, the general tight-binding Hamiltonian for a bilayer reads

$$\begin{aligned} H = & -t \sum_{\mathbf{n}, \boldsymbol{\delta}} (a_{1\mathbf{n}+\boldsymbol{\delta}}^{\dagger} b_{1\mathbf{n}} + h.c.) - t \sum_{\mathbf{n}, \boldsymbol{\delta}'} (a_{2\mathbf{n}}^{\dagger} b_{2\mathbf{n}+\boldsymbol{\delta}'} + h.c.) \\ & + \gamma_1 \sum_{\mathbf{n}} (a_{2\mathbf{n}}^{\dagger} b_{1\mathbf{n}} + h.c.) + \gamma_3 \sum_{\mathbf{n}, \boldsymbol{\delta}'} (a_{1\mathbf{n}}^{\dagger} b_{2\mathbf{n}+\boldsymbol{\delta}'} + h.c.), \\ & - \frac{1}{2} \Delta \sum_{\mathbf{n}} (a_{1\mathbf{n}+\boldsymbol{\delta}}^{\dagger} a_{1\mathbf{n}+\boldsymbol{\delta}} + b_{1\mathbf{n}}^{\dagger} b_{1\mathbf{n}} - (1 \rightarrow 2)), \end{aligned} \quad (3)$$

where t is the in-plane hopping parameter, and γ_1 the strongest inter-layer coupling. When $\Delta = 0$ this Hamiltonian is equivalent to the Slonzewski-Weiss-McClure (SWM) model^{32,33} for the bulk graphite, provided that one retains only in-plane and γ_1 out-of-plane hopping, and assumes no dispersion along the c axis (perpendicular to the planes)³⁴. As mentioned above, the connected sites A2 and B1 lie directly below and above each other, so that the magnetic field perpendicular to the bilayer does not affect this coupling. This is not the case for the weaker A1 – B2 coupling γ_3 included in the Hamiltonian (3) for completeness. In what follows, however, we will neglect this term, whose role is negligible as far as the longitudinal optical sum rule is concerned. Finally, the parameter Δ represents the asymmetry of the on-site energies on the two layers, and it is induced by the electric field applied perpendicular to the graphene bilayer. As we shall see below, it is responsible of the splitting of the valence and conduction bands.

The Hamiltonian (3) describes four bands^{21,25,26,30} $\varepsilon_{\pm}^{(\alpha)}(\mathbf{k})$, $\alpha = 1, 2$ with

$$\begin{aligned} \varepsilon_{\pm}^{(\alpha)}(\mathbf{k}) &= \pm \sqrt{\frac{\gamma_1^2}{2} + \frac{\Delta^2}{4} + |\phi(\mathbf{k})|^2 + (-1)^{\alpha} \Gamma}, \\ \Gamma &= \sqrt{\frac{\gamma_1^4}{4} + |\phi(\mathbf{k})|^2 (\gamma_1^2 + \Delta^2)}, \end{aligned} \quad (4)$$

where the function $\phi(\mathbf{k}) = -t \sum_{\boldsymbol{\delta}_i} e^{i\mathbf{k}\boldsymbol{\delta}_i} = -t \sum_{\boldsymbol{\delta}'_i} e^{-i\mathbf{k}\boldsymbol{\delta}'_i}$. By expanding $\phi(\mathbf{k})$ around the two inequivalent \mathbf{K}, \mathbf{K}' points in the Brillouin zone one gets the usual linear dependence, $|\phi(\mathbf{k})| \approx \hbar v_F |k|$, where the wave-vector \mathbf{k}

is measured from \mathbf{K} points and $v_F = \sqrt{3}ta/(2\hbar)$ is the Fermi velocity, with a the lattice constant ($\mathcal{V} = \sqrt{3}a^2/2$). Using this form, one can easily see from Eq. (4) that at large momenta the four bands reproduce the two Dirac cones $|\varepsilon_{\pm}^{(\alpha)}| = \hbar v_F k \equiv |p|$ of each uncoupled layer. The low-energy band dispersion is, however, drastically affected by the interplane hopping γ_1 and the asymmetry parameter Δ . Indeed, at $\Delta = 0$ for $|\varepsilon_{\pm}^{(1)}| < \gamma_1/4$ the two low-energy bands are parabolic with the dispersion $\varepsilon_{\pm}^{(1)} \approx \pm \hbar^2 k^2/2m$, where the effective mass $m = \gamma_1/(2v_F^2)$, and touch each other as in a semimetal (see Fig. 1a, where we used $t = 3.1$ eV, $\gamma_1 = 0.4$ eV^{26,30}). However, when $\Delta \neq 0$ the system becomes a semiconductor with a gap $\tilde{\Delta} = \Delta\gamma_1/\sqrt{\gamma_1^2 + \Delta^2}$ at the momentum $p_m/\hbar v_F$, that corresponds to the energy $p_m^2 = (\Delta^2/2)(\gamma_1^2 + \Delta^2/2)/(\gamma_1^2 + \Delta^2)$, see Fig. 1b.

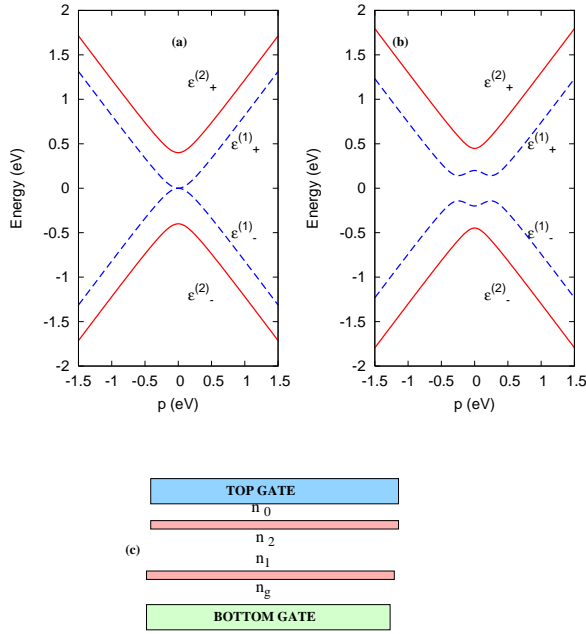


FIG. 1: (Color online) Top: bilayer band dispersion for $\Delta = 0$ (a) and $\Delta = 0.4$ eV (b) as a function of $p \equiv \hbar v_F k$. Bottom: general scheme of the experimental setup for a tunable-gap bilayer device (notation defined in the text).

Although the linear approximation for $\phi(\mathbf{k})$ is sufficient for the analysis of the low-energy band structure and for the numerical study of the mass tensor (9) below, the derivation of this tensor must be done using an unexpanded expression for $\phi(\mathbf{k})$.²⁴ It follows from the definition (2) that (the factor 2 accounts for the spin)

$$\tau_{xx} = \frac{2}{\hbar^2 N} \sum_{\mathbf{k}} \left[(a_{1\mathbf{k}}^+ b_{1\mathbf{k}} + a_{2\mathbf{k}}^+ b_{2\mathbf{k}}) \frac{\partial^2 \phi^*(\mathbf{k})}{\partial k_x^2} + h.c. \right], \quad (5)$$

where we kept the full momentum dependence of $\phi(\mathbf{k})$ (N is the number of unit cells). The thermal average $\langle \tau_{xx} \rangle$ is calculated from the imaginary time Green's

function (GF) $G = -\langle T_\tau \Psi \Psi^\dagger \rangle$, where we introduced $\Psi^+ = (a_{1\mathbf{k}}^+, b_{2\mathbf{k}}^+, a_{2\mathbf{k}}^+, b_{1\mathbf{k}}^+)$. Then the averages $\langle a_{1\mathbf{k}}^+ b_{1\mathbf{k}} \rangle$ and $\langle a_{2\mathbf{k}}^+ b_{2\mathbf{k}} \rangle$ are

$$\begin{aligned} \langle a_{1\mathbf{k}}^+ b_{1\mathbf{k}} \rangle &= T \sum_{i\omega_n} e^{-i\omega_n 0^+} \hat{G}_{41}(i\omega_n, \mathbf{k}), \\ \langle a_{2\mathbf{k}}^+ b_{2\mathbf{k}} \rangle &= T \sum_{i\omega_n} e^{-i\omega_n 0^+} \hat{G}_{23}(i\omega_n, \mathbf{k}), \end{aligned} \quad (6)$$

where $i\omega_n$ is the fermionic Matsubara frequency. The corresponding elements \hat{G}_{41} and \hat{G}_{23} of the GF \hat{G} can be found from the inverse GF²¹

$$\hat{G}^{-1}(i\omega_n, \mathbf{k}) = \begin{pmatrix} z + \frac{1}{2}\Delta & 0 & 0 & -\phi^*(\mathbf{k}) \\ 0 & z - \frac{1}{2}\Delta & -\phi(\mathbf{k}) & 0 \\ 0 & -\phi^*(\mathbf{k}) & z - \frac{1}{2}\Delta & -\gamma_1 \\ -\phi(\mathbf{k}) & 0 & -\gamma_1 & z + \frac{1}{2}\Delta \end{pmatrix} \quad (7)$$

with $z = i\omega_n + \mu$. Then

$$\hat{G}_{41}(i\omega_n, \mathbf{k}) = \frac{\phi(\mathbf{k})[-|\phi(\mathbf{k})|^2 + (\Delta/2 - z)^2]}{[z^2 - (\varepsilon^{(1)})^2][z^2 - (\varepsilon^{(2)})^2]}, \quad (8)$$

and $\hat{G}_{23} = \hat{G}_{41}(-\Delta)$. Calculating the Matsubara sum in Eq. (6) and using the identity $\phi(\mathbf{k})(\partial^2 \phi^*(\mathbf{k})/\partial k_\alpha^2) + c.c. = -(a^2/3)|\phi(\mathbf{k})|^2$, we finally obtain

$$\frac{\langle \tau_{xx} \rangle}{\mathcal{V}} = -\frac{2a^2}{3\hbar^2 \mathcal{V} N} \sum_{\mathbf{k}, \lambda=\pm, \alpha} |\phi(\mathbf{k})|^2 f(\varepsilon_\lambda^{(\alpha)}(\mathbf{k}) - \mu) M(\varepsilon_\lambda^{(\alpha)}(\mathbf{k})), \quad (9)$$

where

$$M(\varepsilon_\lambda^{(\alpha)}(\mathbf{k})) = \left[\frac{1}{2} + (-1)^\alpha \frac{\gamma_1^2 + \Delta^2}{4\Gamma} \right] \frac{1}{\varepsilon_\lambda^{(\alpha)}(\mathbf{k})} \quad (10)$$

and $f(\varepsilon) = 1/[\exp(\varepsilon/T) + 1]$ is the Fermi distribution. One can verify that for $\gamma_1 = \Delta = 0$ Eq. (9) reduces to the doubled one-layer sum of Ref. [24].

The expression (9) does not show any clear formal resemblance to the kinetic-energy density of the bilayer system, that one would define using the bands (4) as:

$$K = \frac{2}{\mathcal{V} N} \sum_{\mathbf{k}, \lambda=\pm, \alpha} \varepsilon_\lambda^{(\alpha)}(\mathbf{k}) f(\varepsilon_\lambda^{(\alpha)}(\mathbf{k}) - \mu). \quad (11)$$

Nonetheless, as we shall see these two quantities show approximately the same doping dependence, satisfying again the general relation between sum rule and kinetic energy, despite the complicated band evolution with doping of the bilayer system.

III. SUM RULE AS A FUNCTION OF DOPING

As we already mentioned, it was shown experimentally²⁶⁻²⁸ that one can tune independently the asymmetry gap Δ between the two layers and the total carrier density (the value of μ). This corresponds

to controlling the excess carrier density $n_{1,2}$ (difference between the densities of electrons and holes) in each layer as schematically shown in Fig. 1c. The charge on the surfaces below the bottom layer and above the top layer is n_g and n_0 , respectively. In the experimental configuration of Ref. 26 n_g is varied by changing the gate voltage and n_0 by chemical deposition of dopants on top of the upper layer (see also Ref. 27), while in the device of Ref. 28 both n_0 and n_g are varied, by using two independent gates. The resulting asymmetry Δ between on-site energies in the two layers can be determined by equating the voltage difference Δ/e between the plates of the capacitor to its value evaluated from the charge density $e(n_0 + n_2 - n_g - n_1)$.^{21,26,30}

$$\Delta = \frac{e^2 d}{2\epsilon_0} [n_0 + n_2(\Delta) - n_g - n_1(\Delta)] = \frac{n_0 e d}{\epsilon_0} + \frac{n_2(\Delta) e d}{\epsilon_0}. \quad (12)$$

Here d is the bilayer thickness, ϵ_0 is the permittivity of free space and in the last equality we used that the total carrier excess $n = n_1 + n_2 = -(n_0 + n_g)$. Since $n_1(\Delta = 0) - n_2(\Delta = 0) = 0$, we obtain that $\Delta = 0$ at $n = -2n_0$. The gap closes when the system is doped away from half-filling, as indicated by the ARPES measurements of Ref. 27. However, if the value of n_0 is tuned to be exactly at zero²⁸, the gap closes exactly at the neutrality point, where the semimetal band structure is reproduced. For finite Δ the excess carrier densities $n_{1,2}$ are given by

$$n_1(\Delta, \mu) = \frac{1}{NV} \sum_{\mathbf{k}, \alpha} [f(\epsilon_+^{(\alpha)}(\mathbf{k}) - \mu) - f(\epsilon_+^{(\alpha)}(\mathbf{k}) + \mu) + g^{(\alpha)}(\mathbf{k}) [f(\epsilon_-^{(\alpha)}(\mathbf{k}) - \mu) - f(\epsilon_-^{(\alpha)}(\mathbf{k}) + \mu)]], \quad (13)$$

where $g^{(\alpha)}(\mathbf{k}) = (\Delta/\epsilon_+^{(\alpha)}(\mathbf{k}))(1/2 + (-1)^\alpha |\phi(\mathbf{k})|^2/\Gamma)$, and $n_2(\Delta, \mu) = n_1(-\Delta, \mu)$. To determine selfconsistently the dependence Δ on n , one has to solve simultaneously Eq. (12) and the equation $n_1(\Delta, \mu) + n_2(\Delta, \mu) = n$ for the chemical potential μ . Once $\Delta(n)$ and $\mu(n)$ are determined, one can compute $\langle \tau_{xx} \rangle$ and K as a function of n .

Following Ref. 27 we use $d = 3.4 \text{ \AA}$, and show results for $n_0 = 0, n_0 = \pm 12 \times 10^{12} \text{ cm}^{-2}$. This choice is suggested by the fact that in the measurements of Ref. 27 the gap closes at $n = -2n_0$ given approximately by $24 \times 10^{12} \text{ cm}^{-2}$ (notice that n expressed in units of 10^{12} cm^{-2} corresponds to $1.9 \times 10^3 n_{uc}$, where n_{uc} is the number of electrons per unit cell n_{uc}). The doping dependence of the $\langle \tau_{xx} \rangle$ at $T = 0$ is shown in Fig. 2. As one can see, even though the charging gap Δ changes consistently with doping (see inset of Fig. 2), due to the screening effects of the bilayer device, nonetheless the sum rule attains overall variations of $\sim 0.1\%$, which are undetectable from an experimental point of view. In other words, despite the large optical-conductivity spectral-weight redistribution associated with the opening of the

gap through the semimetal-semiconductor transition induced by doping, the sum rule is not affected. It follows the same behavior that one would obtain in (electrostatically) uncoupled layers where $\Delta = 0$ at all doping (see the dashed-dotted line in Fig. 2). In the regime where the gap is relatively small (for example at negative doping for the $n_0 = 12 \times 10^{12} \text{ cm}^{-2}$ curve in Fig. 2) the sum rule follows approximately the same doping dependence found in the single-layer case, i.e. $[\tau_{xx}(n) - \tau_{xx}(0)]/\mathcal{V} \simeq -2a^2|\mu|^3/(9\pi\hbar^2 v_F^2)$. Since $2a^2/(9\pi\hbar^2 v_F^2) \approx 10^{-2} \text{ eV}^{-2}$, and $|\mu|^3$ has an overall variation of at most $0.1(\text{eV})^3$ in the considered doping range, one can easily get the small sum-rule variation with doping. At larger gap values, $\tau_{xx}(n) - \tau_{xx}(0)$ is slightly larger than expected in the single-layer case, but is still too small to be detected experimentally. As far as the temperature dependence is concerned we always found a $(T/t)^2$ variation, as expected due to the parabolic structure of the low-energy bands. Including other hoppings such as γ_3 in the Hamiltonian (3) can change the dispersion curve as discussed in²⁹ (see also Ref. 34) for energies less than 2 meV. While this can slightly affect the overall value of the optical integral and of the self-consistent Δ , it does not change the main conclusion of our calculation, which focus on the relative doping changes of the sum rule when a large semiconducting gap Δ of order of a few hundred meV is opened. Having established that the relatively large band-structure changes caused by the opening of the gap Δ lead to a negligible changes in the optical sum, we expect that the above mentioned hopping terms introduce negligible corrections as well.

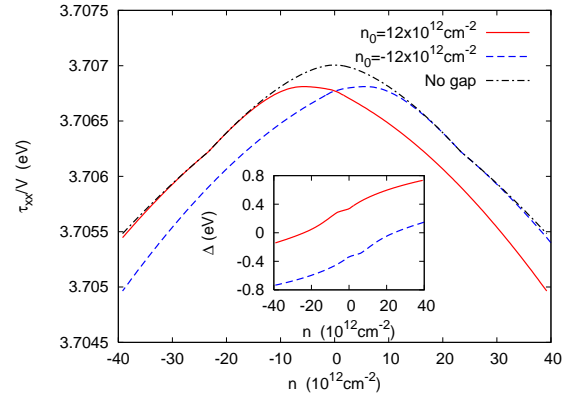


FIG. 2: (Color online) Doping dependence of the $T = 0$ sum rule for a bilayer system with a doping-dependent gap $\Delta(n)$, shown in the inset. We show results for different values of n_0 , given in units of 10^{12} cm^{-2} . For comparison, we show the equivalent doping dependence of the sum rule when no gap is present between the two layers (dashed-dotted line).

Analogously, the kinetic energy, shown in Fig. 3, is not much affected by the opening of the gap, and it attains a value which is approximately 6 times the sum rule, $\tau/\mathcal{V} \sim (1/6)|K|$. There are however two differences in the doping dependence of the sum rule with respect to the kinetic energy. First, we notice that the very small

changes in the sum rule and kinetic energy have the opposite trend: indeed, they both decrease when the gap opens, in contrast to what is found for example at the transition between a normal metal and a superconductor, where a kinetic-energy increase corresponds to a sum-rule decrease and vice-versa. This effect disappears when we set $\gamma_1 = \Delta = 0$ in our numerical work: indeed, in this case τ_{xx} reproduces exactly twice the single-layer value computed in Ref. [24], and the sum rule and the kinetic energy track each other exactly as the doping is varied. Second, it is clear from Fig. 3 that the chemical-potential jump at the neutrality point in the biased case (see inset (b) of Fig. 3) is much more effective on the kinetic-energy doping dependence. The two curves for $|K|$ at $n_0 = \pm 12 \times 10^{12} \text{cm}^{-2}$ in Fig. 3 show a kink at $n = 0$ which is clearly due to the $\mu(n)$ discontinuity at the neutrality point. Indeed, in the case where no gap is present in the system $\mu(n)$ goes smoothly across $n = 0$, as does the kinetic energy. Instead, the sum-rule curves in Fig. 2 are not much affected by the μ discontinuity at $n = 0$.

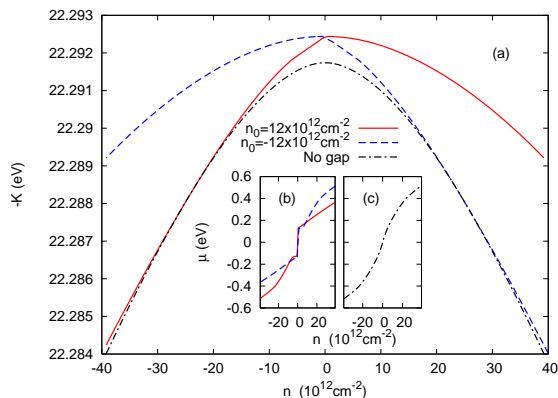


FIG. 3: (Color online) (a) Doping dependence of the $T = 0$ kinetic energy for a bilayer system with a doping-dependent gap $\Delta(n)$ and without it. Observe the small variations of K in the considered doping range. Insets: doping dependence of the chemical potential when a gap is present (b) or not (c), for parameters as in the main frame.

IV. CONCLUSIONS

In summary we investigated the behavior of the optical sum in bilayer graphene as a function of charge imbalance carrier density n and temperature. While a small temperature variation could be expected because of the relatively small effect of temperature on the elec-

tronic excitations, the negligible dependence of the sum rule on the carrier density was not a priori expected. Indeed, despite the profound band-structure changes induced by the change of doping, no significant signature appears on the overall spectral weight. This implies that the spectral weight lost in the gap must appear above it, and the two must largely compensate for each other. Observe that in order to be able to test experimentally such a prediction one would need to define an “experimental” cut-off. Indeed, even though the relation (1) is theoretically established by integrating the optical conductivity to all frequencies, in practice an intrinsic cut-off is provided by the frequency ω_c above which transitions to other electronic bands not considered in the present study would develop.² According to optical studies on graphite³⁵, the optical sum rule saturates to the value corresponding to one electron per atom (as due to the π band considered here) around 8 eV, while optical transitions coming from the σ bands appear around 15 eV. However, in the present case a much smaller cut-off could be used, if one wants just to compare the spectral-weight variations induced by the opening of the gap. Indeed, the spectral-weight redistribution is expected to fall in a range of frequencies of order 2Δ , as confirmed recently in Ref.²². Thus, an upper cut-off of order of $\omega_c \simeq 1 - 2$ eV should be enough to account for the gap-opening effects, and to test experimentally the predicted robustness of the optical sum rule.

It is worth noting that in our calculation only the electrostatic interaction between layers was included, since this is believed to be the most important effect in the system. However, as in the case of cuprates superconductors other mechanisms (electron repulsion or electron-phonon interactions) could be at play and modify the sum rule. Thus, the experimental verification of our prediction would help understanding if other interactions need or need not be taken into account in dealing with these systems.

Acknowledgments

Useful discussions with V.P. Gusynin, A.B. Kuzmenko and E.J. Nicol are acknowledged. J.P.C. and S.G.Sh. were supported by the Natural Science and Engineering Research Council of Canada (NSERC) and by the Canadian Institute for Advanced Research (CIFAR). L.B. acknowledges partial financial support from Miur PRIN 2005, Prot. 2005022492.

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